

Fig. 1

Performance Characteristics

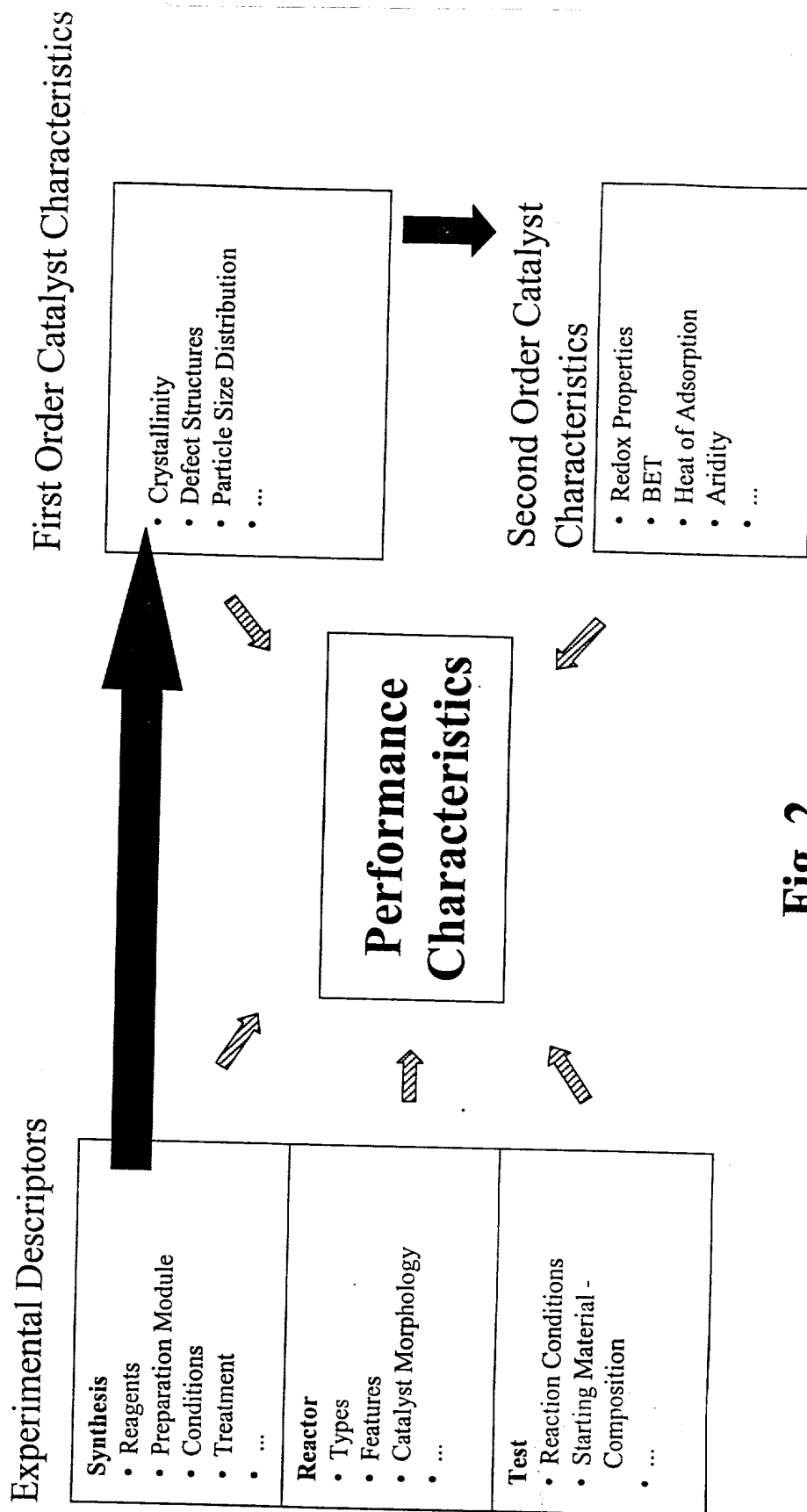


Fig. 2

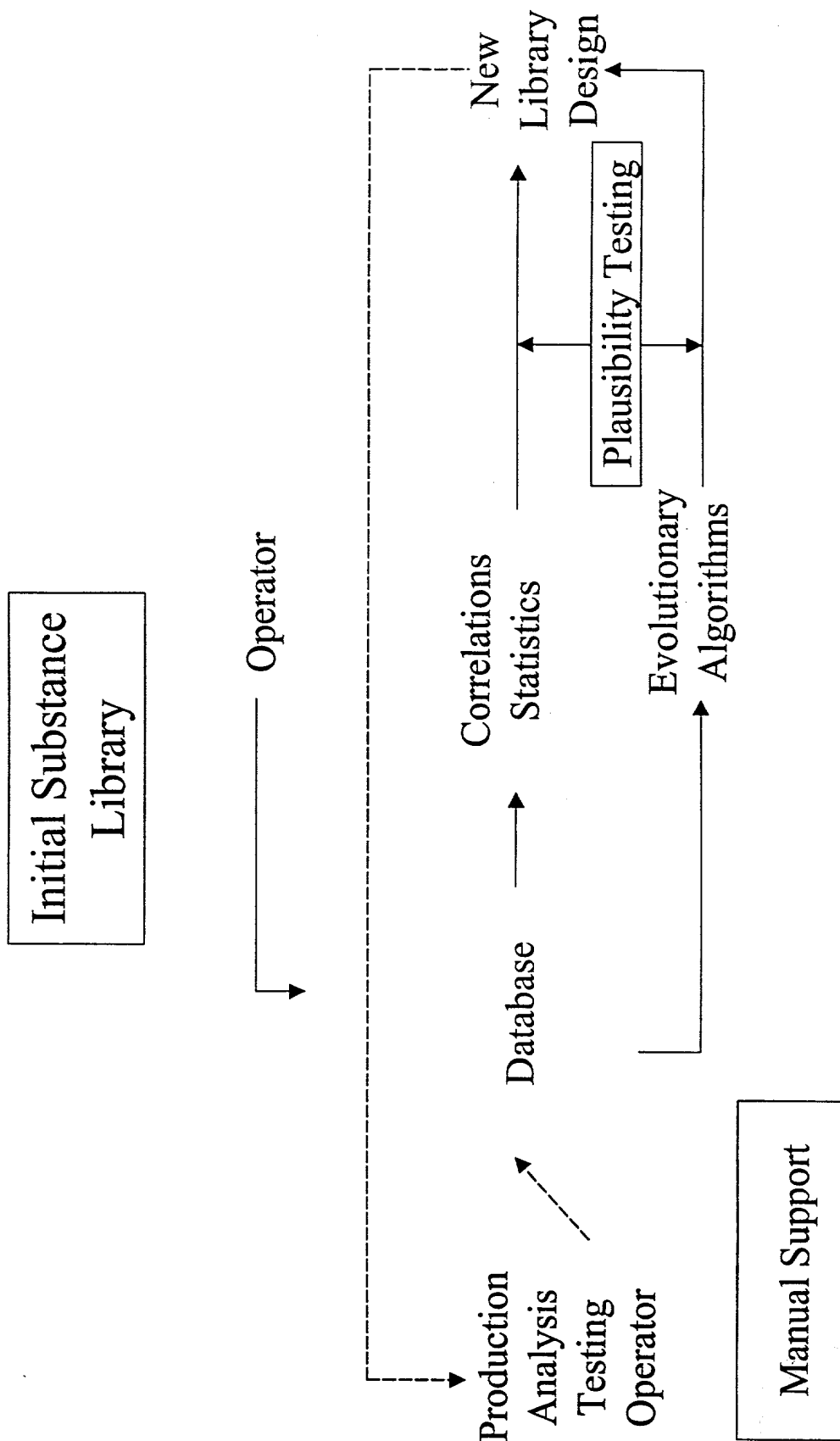


Fig. 3

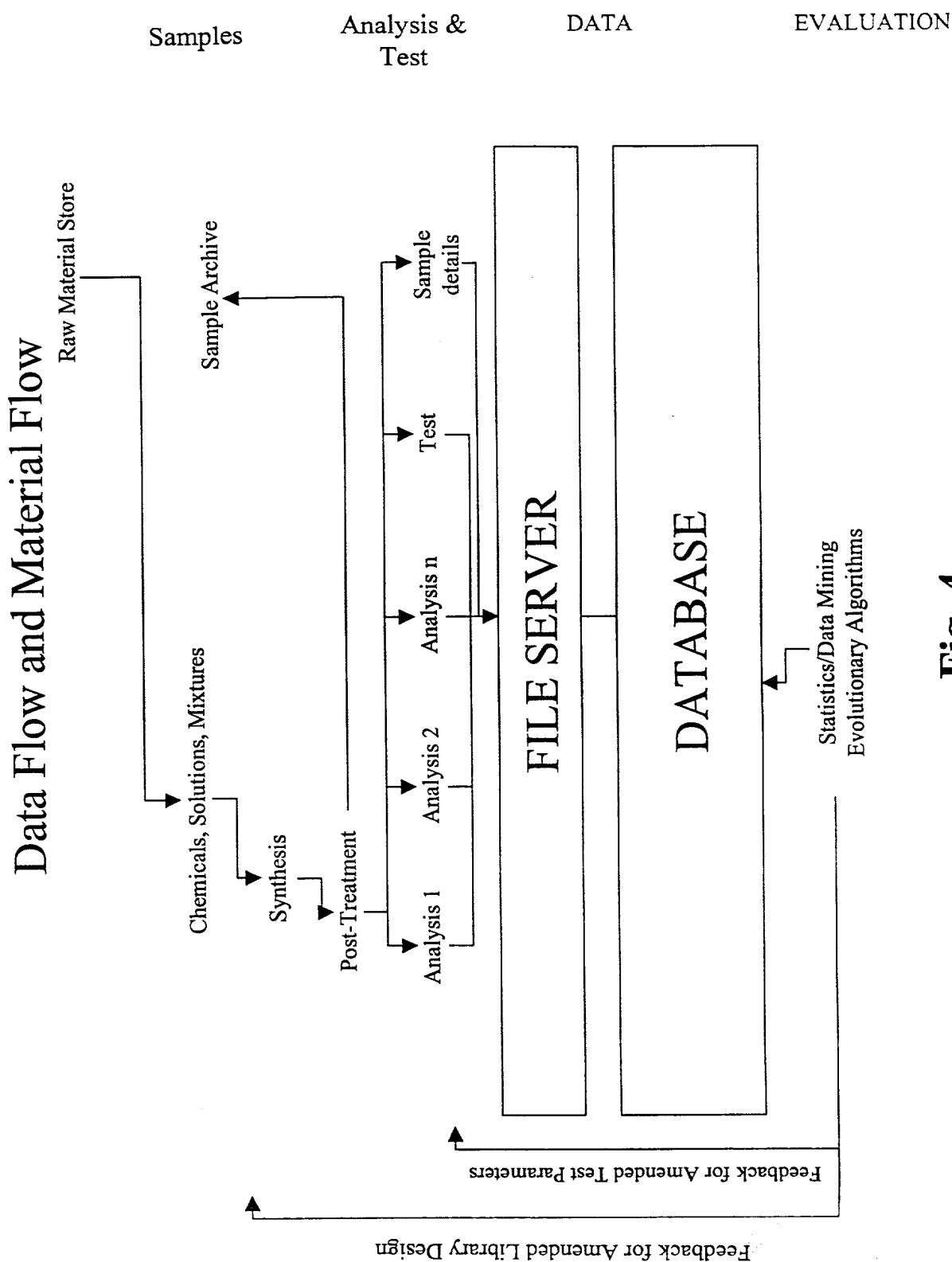
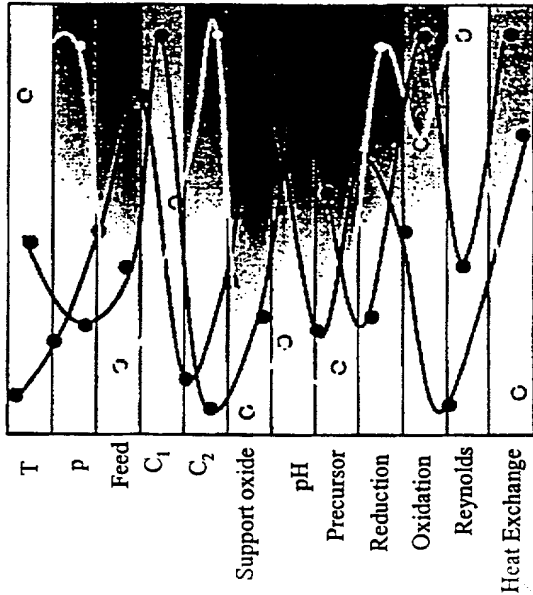


Fig. 4

Original Library Design and Tests Using the Entire Parameter Space

Step 1: Design of Library, Test
and Process Conditions



Step 2: Data Acquisition

	Experiment 1	Experiment 2	Experiment n
T	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
p	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Feed	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
C ₁	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
C ₂	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Support oxide	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
pH	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Precursor	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Reduction	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Oxidation	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Reynolds	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Heat Exchange	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Activity	++	+	++
Selectivity	+	++	-

Fig. 5a

Regression Analysis, Energies of the Parameter Space

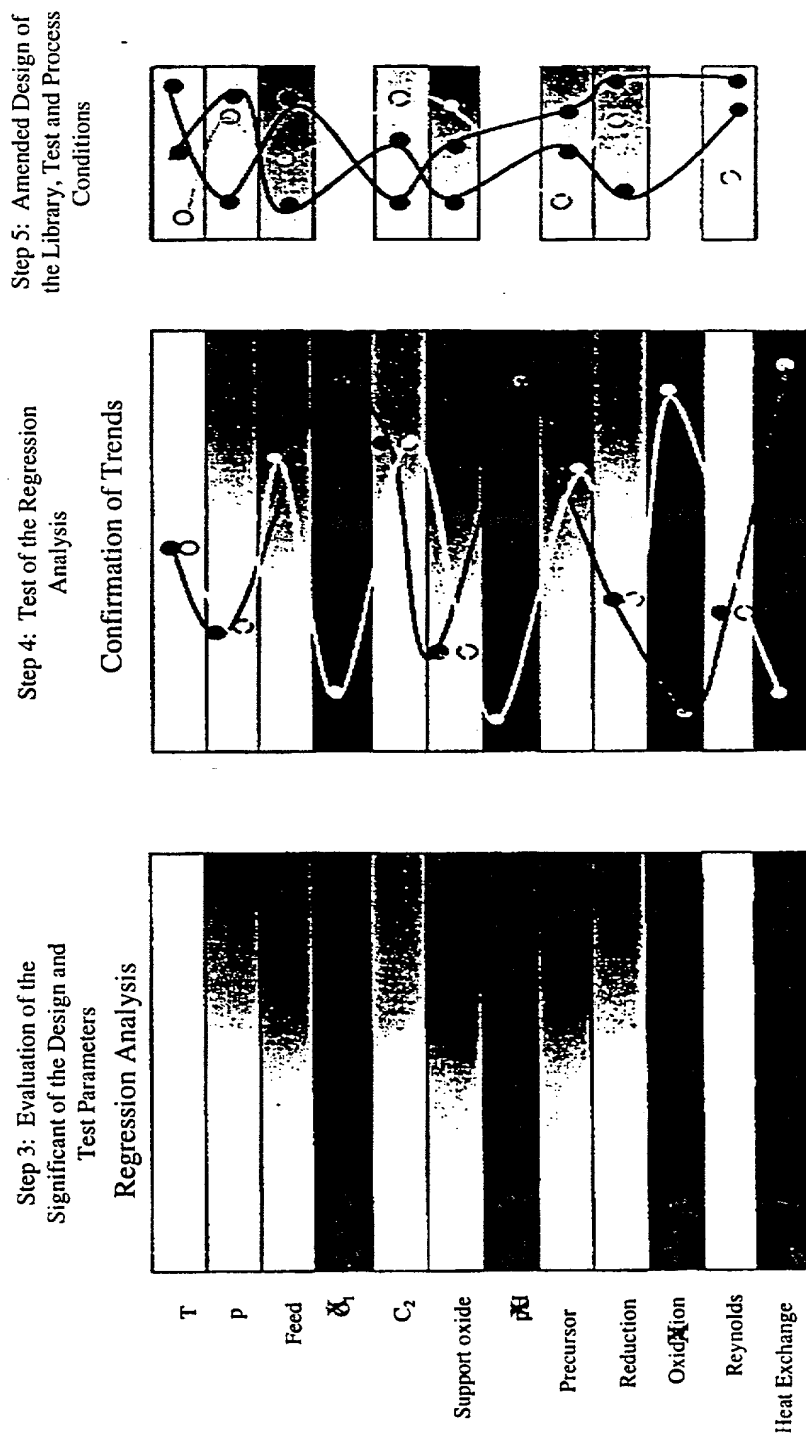


Fig. 5b

Principle of Genetic Algorithms

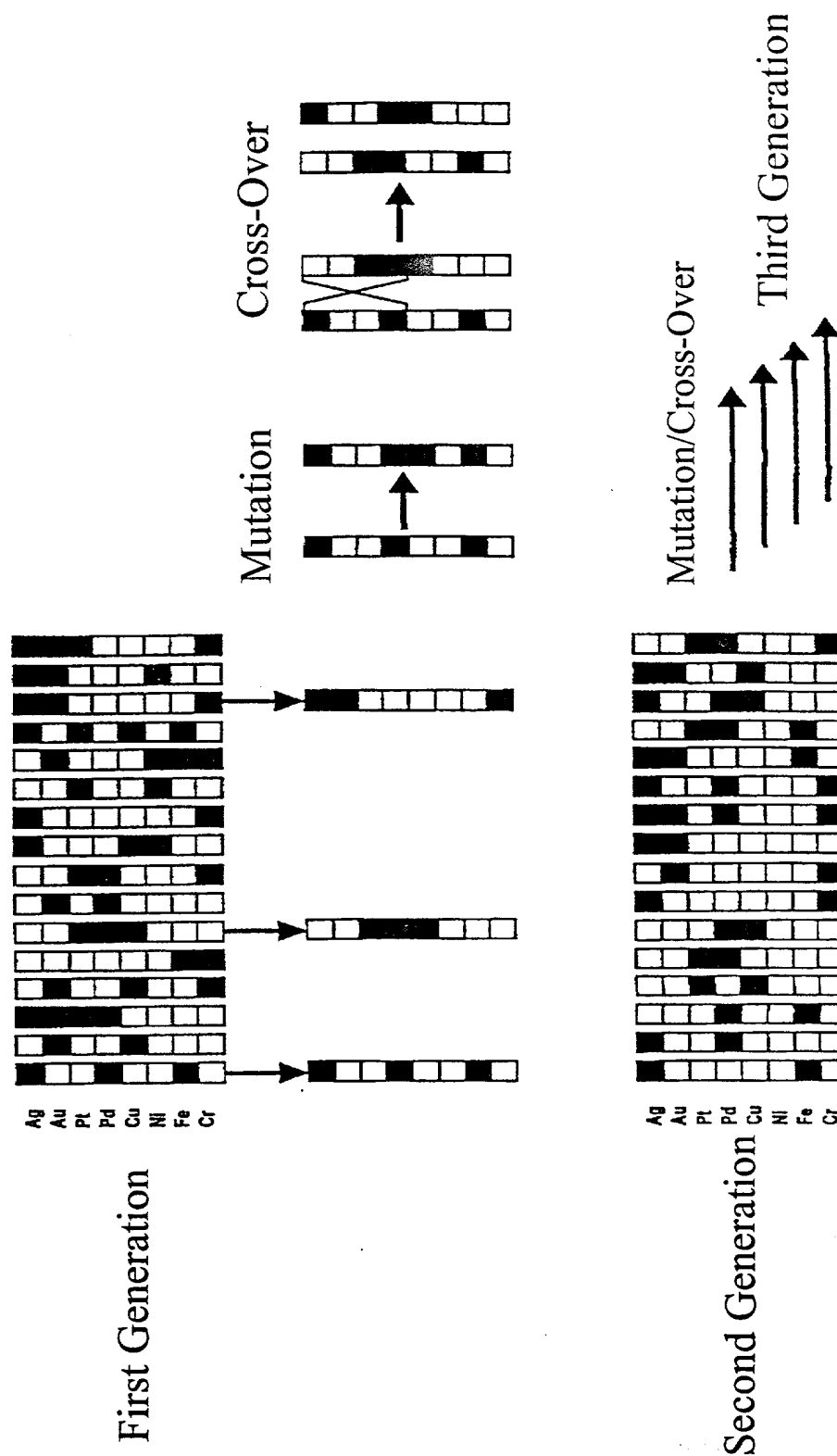


Fig. 5c

Sensitivity Analysis of the Parameters of the Initial Library Pareto Diagram

Pareto Chart of Standardized Effects; Variable: U_NOX
7 factors, 5 Blocks, 96 Runs; MS Residual=128,2875
DV: U_NOX

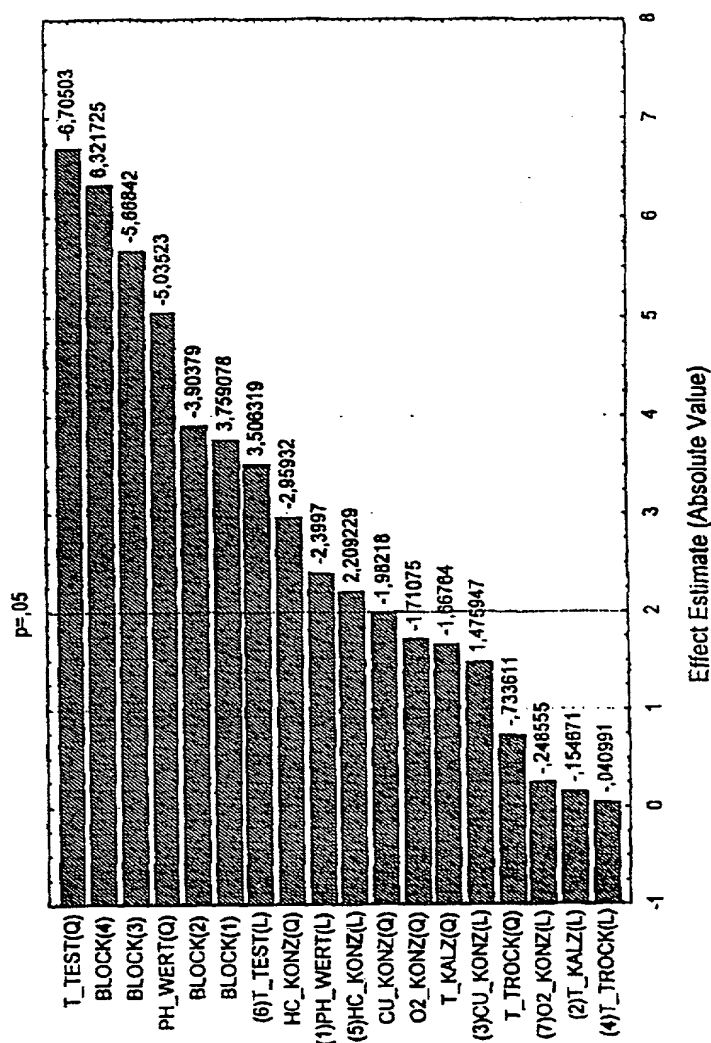


Fig. 6

Sensitivity Analysis of the Parameters of the 1st Optimized Library Pareto Diagram

Title: COMPUTER-AIDED
OPTIMIZATION OF SUBSTANCE
LIBRARIES
Inventor(s): Stephan SCHUNK et al
Appl. No.: 09/876,142

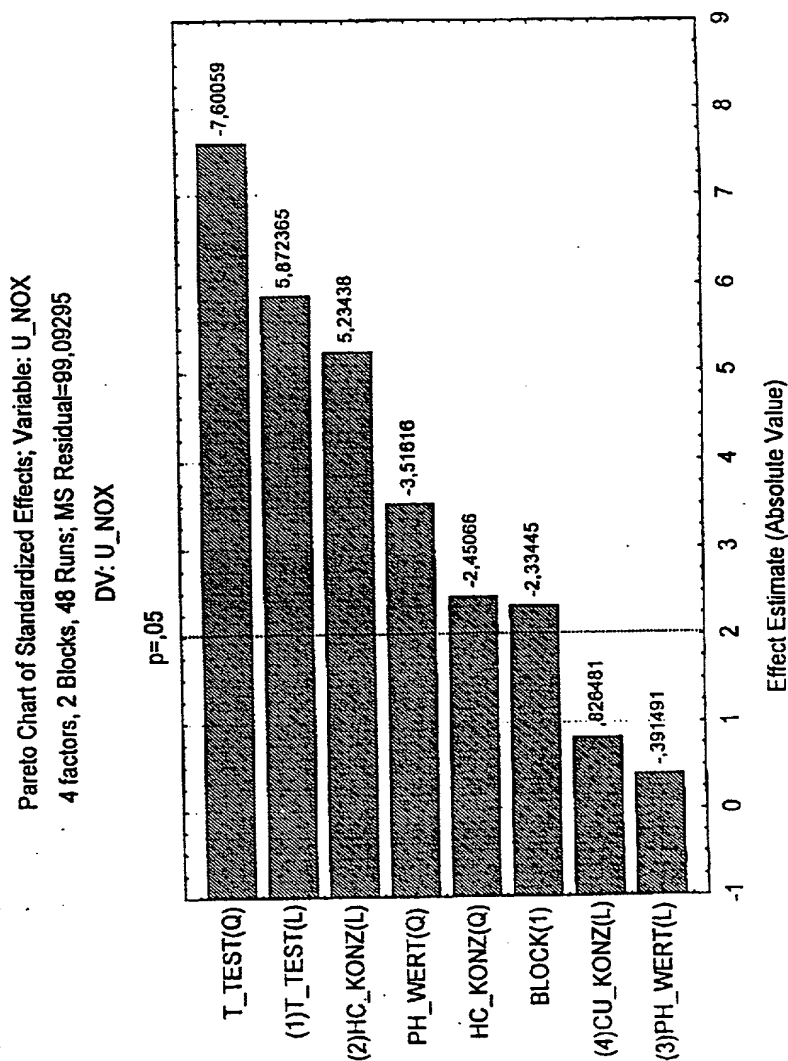


Fig. 7